Efficient quantum measurement of Pauli operators in the presence of finite sampling error

Ophelia Crawford, Barnaby van Straaten, Daochen Wang, Thomas Parks, Earl Campbell, Stephen Brierley

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Estimating the expectation value of an operator corresponding to an observable is a fundamental task in quantum computation. For example, expectation estimation of a Hamiltonian features prominently as the quantum subroutine of the variational quantum eigensolver (VQE) algorithm [1]. It is often impossible to obtain such estimates directly, as the computer is restricted to measuring in a fixed computational basis. One common solution splits the operator into a weighted sum of Pauli operators and measures each separately, at the cost of many measurements. An improved version collects mutually commuting Pauli operators together before measuring all operators within a collection simultaneously. The effectiveness of doing this depends on two factors. Firstly, we must understand the improvement offered by a given arrangement of Paulis in collections. Secondly, to measure all Pauli operators within a collection simultaneously, a circuit, U, is required to rotate them to the computational basis. Recently, a series of papers [2–8] have appeared that together make good progress on both the collecting strategy and rotation circuit construction problems. Our paper is in this same arena and addresses both problems.

We first consider the arrangement of Pauli operators into commuting collections. We define two metrics, R and $\hat{R}$, that quantify the performance of any given arrangement. R and $\hat{R}$ give the ratio of the number of measurements required in the uncollected case to the collected case to attain a fixed level of accuracy, assuming measurements are distributed optimally between the collections to minimise the finite sampling error [9–11]. R is state-dependent and $\hat{R}$ is designed to approximate $\mathbb{E}[R]$ over the uniform spherical measure. With R and $\hat{R}$ defined, we prove that breaking a commuting collection into two never reduces the number of measurements required to obtain an expectation estimate to a given level of accuracy. This result contradicts a previous conclusion, demonstrated through a toy example [6, 12], that breaking a collection can be advantageous. The discrepancy is because we distribute measurements optimally among the collections, whereas in the previous works, measurements are distributed uniformly. We then propose a new collecting strategy, "SORTED INSERTION". Unlike all strategies used previously that seek the minimum number of collections [2, 3, 6, 7], SORTED INSERTION attempts to maximise $\hat{R}$ by considering the coefficients of the Pauli operators in its assignment of collections.

Turning to the rotation circuit construction problem, we contribute two new methods, "CZ" and "CNOT", for constructing Clifford circuits, U, that enable simultaneous measurement of a collection of arbitrary commuting Paulis. Like Gokhale et al. [6], we approach the problem via the stabiliser formalism, but further consider the case where the number of independent operators, k, in a collection can be less than the number of qubits, n. We show that the number of two-qubit gates in U can be reduced in a way that scales with k. Furthermore, we allow classical post-processing, which can save quantum resources. Building on work in the graph-state [13] and circuit synthesis [14, 15] literature, we obtain U with numbers of two-qubit gates at most $u_{\text{cz}}(k,n) = kn - k(k+1)/2$ and $u_{\text{cnot}}(k,n) = O(kn/\log k)$ for the CZ- and CNOT-constructions respectively. The sparsity of an extension step that exploits k plays an important role for both formulae.

We end our paper with a series of numerical results on molecular Hamiltonians, ranging in size from H_2, which requires two qubits, to H_2Se, which requires 38. For the nine smallest systems, we calculate the value of R for 100 different random quantum states to quantify the improvement due to assembling the Hamiltonian into collections of commuting operators. In practice, the value of R can at best be obtained approximately by making measurements on the quantum computer and so cannot be used to determine the expected advantage of a particular arrangement a priori. The metric $\hat{R}$, on the other hand, depends only on the coefficients of the terms in the Hamiltonian. We find that $\hat{R}$ closely approximates the average of R over many quantum states for the states we have considered. We therefore propose using $\hat{R}$ as a metric for the quality of a collecting method, and compare different methods of collecting the operators with this metric in mind. Calculating $\hat{R}$ on the full range of molecules shows that our SORTED INSERTION algorithm results in a 10- to 60-fold reduction in the number of measurements required to attain a fixed level of accuracy. We further find that SORTED INSERTION outperforms the four conventional greedy colouring algorithms we tested, as measured by $\hat{R}$. The reduction in the number of measurements required comes at the cost of applying additional quantum gates before the qubits are measured, the most costly of which are two-qubit gates. Using the CZ-construction, for the molecules we have considered, we find that the largest number of two-qubit gates required is far lower than the theoretical maximum, typically by a factor of approximately 3.5.

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